Electron Spin Coherence and Manipulation in Si Quantum Dots

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Major Decoherence Channels of A Confined Electron Spin

Spin Environment:

- Crystal lattice, lattice defects/impurities, nuclear spins, …
- Electronic orbital states, other electron magnetic moments, …

Single Spin States:

- Low temperature to freeze out the orbital degrees of freedom;
- Spin environment from paramagnetic impurities (MOS QDs);
- Hyperfine coupling to nuclear spins + nuclear dynamics;
  - ✓Nuclear dynamics due to magnetic dipole interaction;
  - ✓Nuclear dynamics due to hyperfine interaction;
  - ✓…
- Spin-orbit interaction + electron-phonon interaction;

Hyperfine Interaction for a Conduction Electron in Si

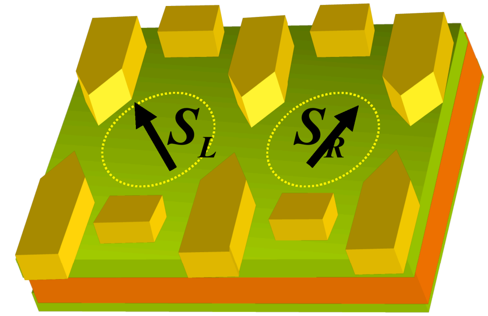
➢Important parameter for both electron spin decoherence and manipulation in Si quantum dots

✓Nuclear spin induced decoherence depends on the strength of hyperfine interaction;
✓Manipulation of two-spin states with inhomogeneous magnetic fields could use the Overhauser field, [for example, Petta et al (2005)].

➢Hyperfine interaction not well characterized theoretically. Not calculation exists for conduction electrons in Si.

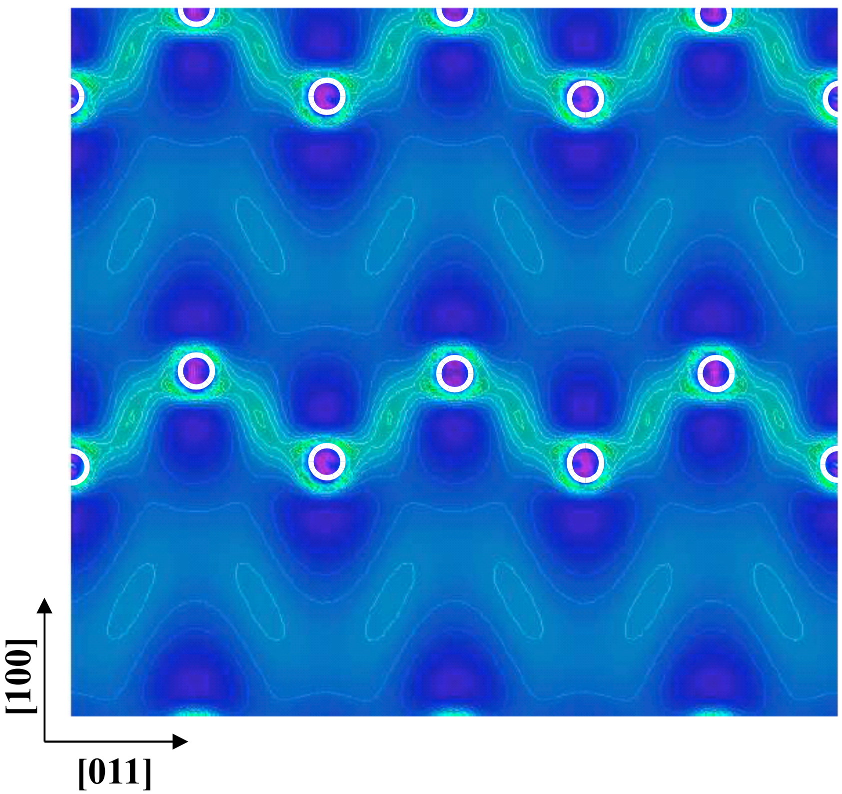
➢Pseudopotential method not reliable near the nuclei;

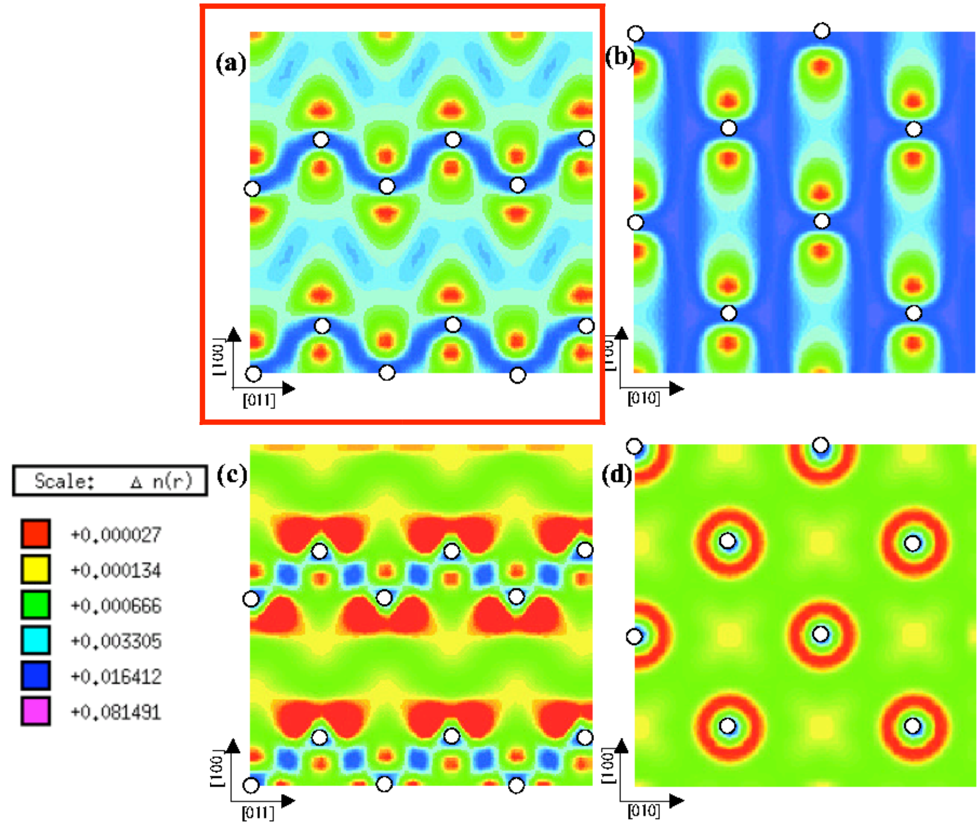
➢**All-electron approach (APW, WIEN2K package)**; Largest supercell size N = 64; Spin-orbit interaction included; Electron interaction described within the density functional framework.



In SiGe heterostructures (Wisconsin, Purdue, Princeton, …) or SiMOSFET (Sandia, UCLA, NTT, UNSW, …)

Spin Density in Singly Negatively Charged Si





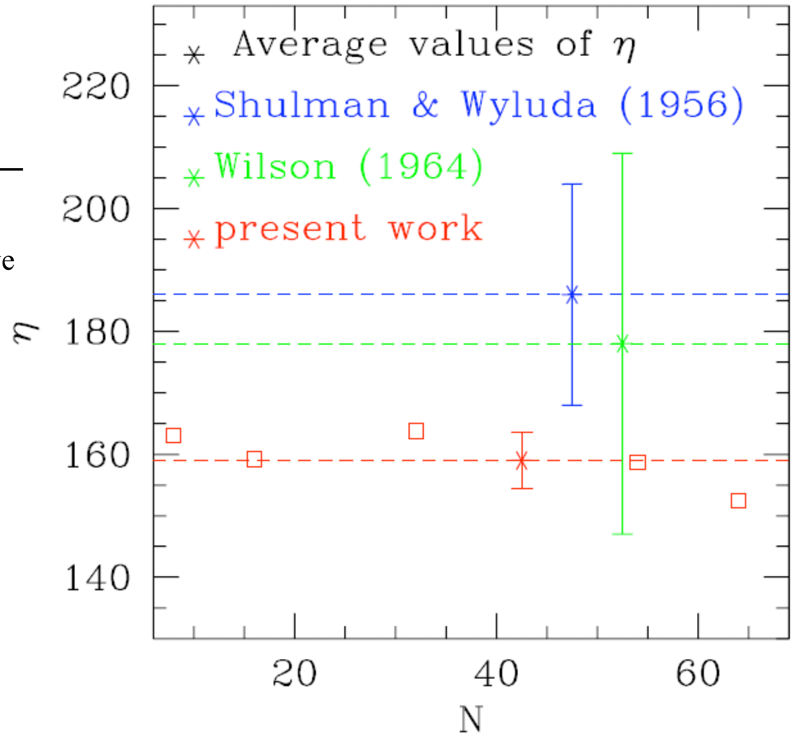
Koiller et al., PRB (2004).

Results in the interstitial region comparable to those obtained with pseudopotential method. On site the electron probability is much higher in the all-electron calculation.

Electronic Probability in the Core Region: Compared to Experimental Measurements

Definition:

$$\eta = \Omega \frac{|\psi(0)|^2}{\left\langle |\psi|^2 \right\rangle_{ave}}$$



For comparison, in GaAs

$$\eta_{Ga} \approx 2700 \text{ and } \eta_{As} \approx 4500$$

With pseudopotential method

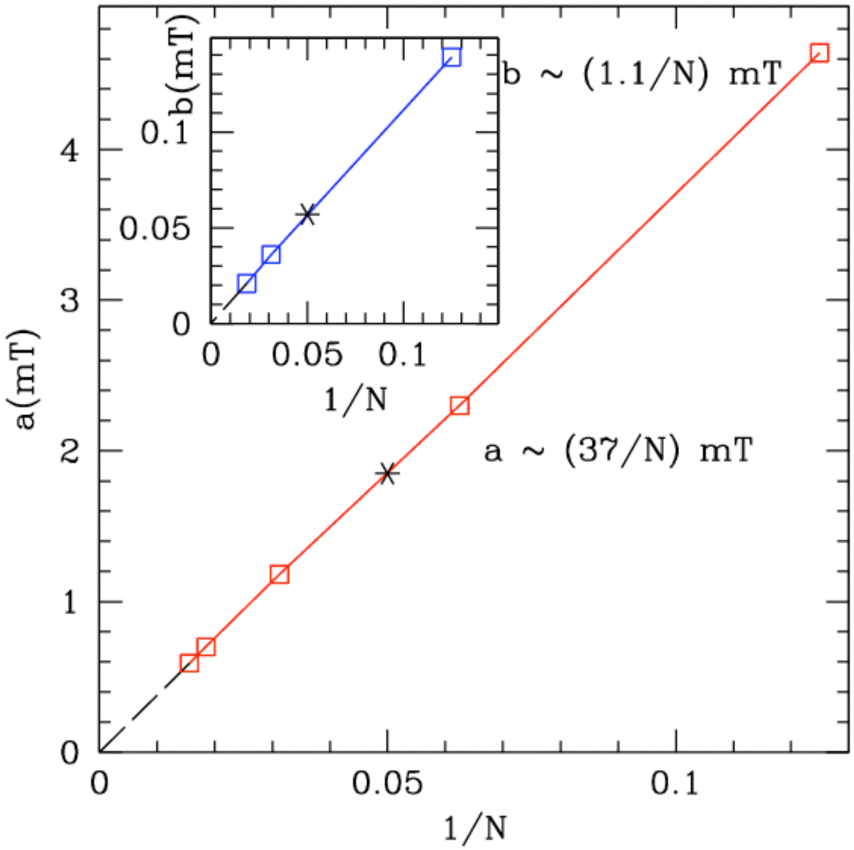
$$\eta_{Si}^{pp} \sim 3$$

Our calculation:

$$\eta_{Si} = 159.4 \pm 4.5$$

- Shulman and Wyluda, Phys. Rev. **103**, 1127 (1956), spin-lattice relaxation measurement $\eta = 186 \pm 18$
- I. Solomon, in D.K. Wilson, Phys. Rev. **134**, A265 (1964), spin-lattice relaxation measurement $\eta = 178$.
- Dyakonov and Denninger, Phys. Rev. B **46**, 5008 (1992), Overhauser field measurement, about twice as large as 180. η value not given.

Hyperfine Interaction Strengths in Si



- "N" size of the supercell. For natural Si, there is about 5% ^{29}Si;
- "a" contact hyperfine strength; $\boxed{a \sim 1.9\ \text{mT}}$ for N = 20.
- "b" anisotropic hyperfine strength when the electron is in a single valley, about 3% of "a".

Hyperfine Interaction in a Quantum Dot: GaAs and Natural Si

	QD size (# of atoms)	# of nuclei with finite spin	Maximum Overhauser field	Random Overhauser field	T_2^*
GaAs	10^6	10^6	100 μeV	0.1 μeV	10 ns
Natural Si	10^6	5×10^4	200 neV	1 neV	1 μs
Natural Si	10^5	5×10^3	200 neV	3 neV	300 ns

The T_2^* time in Si QD will be 1~ 2 orders of magnitude longer than in GaAs!

Major Decoherence Channels of Multiple Trapped Electron Spins

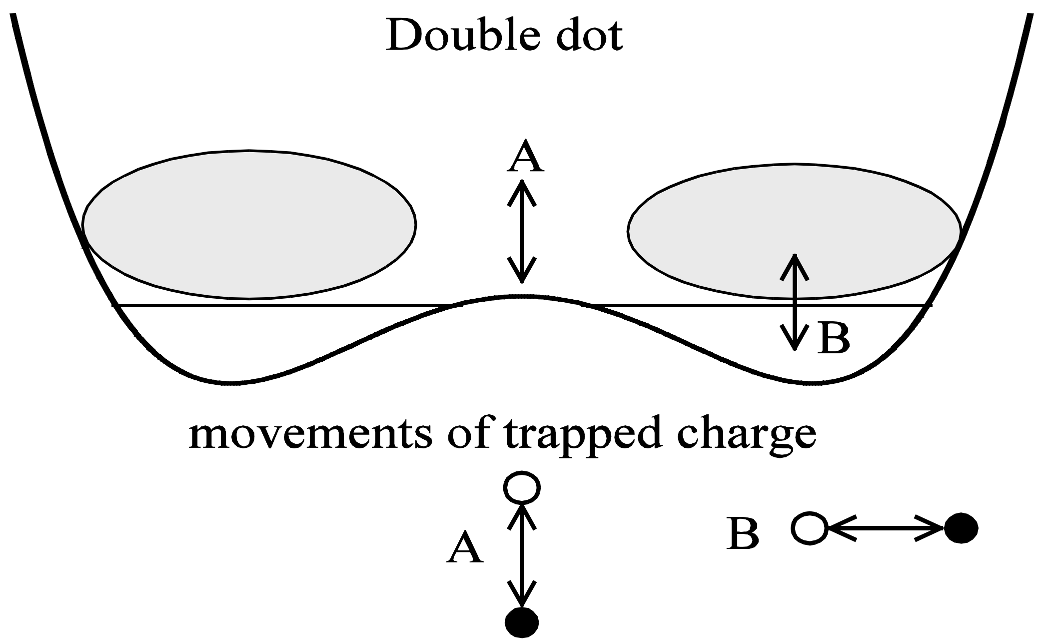
<u>Two-Spin States</u>:

- Factors affecting single spins;
- Gate electrode voltage fluctuations;
- Environmental charge fluctuations;
- Electron-phonon interaction;

If exchange interaction is turned on

How Does Charge Noise Affect an Exchange Coupled Double Dot

Exchange coupling is Coulombic!

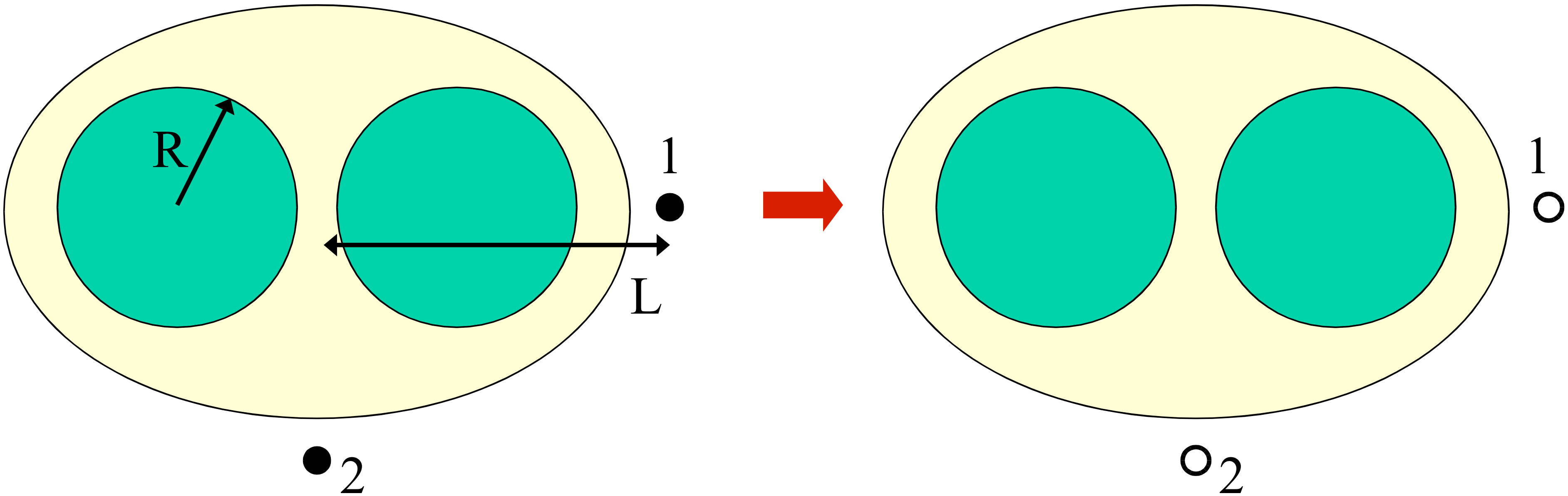


What some charge fluctuations do:

- ➢Vary the interdot barrier;
- ➢Change the bias between the two dots.

Both affect J!

Effects of a Charging and Discharging a Trap in a Symmetric SiMOSFET Double Dot



- Strongly dependent on the trap location;
- Screened by the 2DEG nearby;

For example, for a double dot with R = 8 nm, interdot distance 50 nm, and L = 75 nm, if trap 1 is discharged, the change in the electrostatic potential causes a relative change in exchange coupling of $\delta J/J \sim 10^{-4}$

D. Culcer, X. Hu, and S. Das Sarma, APL **95**, 073102 (2009).

Sensitivity to Gate Noise and Charge Noise For a Biased Double Dot

When the double dot is strongly biased, the exchange splitting is determined by the tunnel coupling between the two-dot and single-dot singlet states and the inter-dot bias:

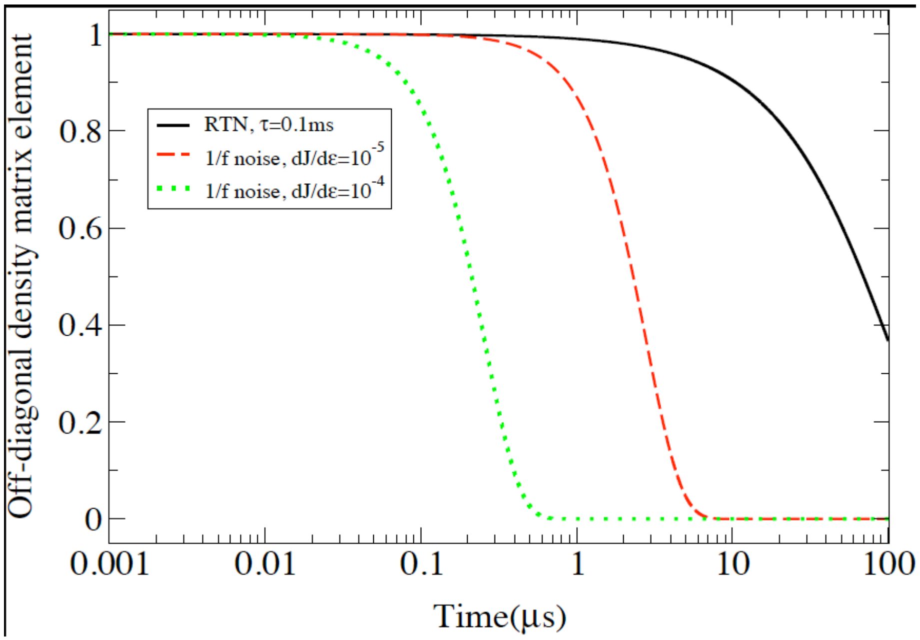
$$J \sim \frac{t^2}{E_b}$$

Where t is the tunnel coupling between the two singlet states, and E_b is the energy difference between these two states, which is dominated by the inter-dot bias. Thus

$$dJ \;\square\; \frac{\square}{\square} dt \;\square\; \frac{J}{E_b} dE_b \;\square\; \frac{J}{E_b} dV_{b1} \;\square\; \boxed{\frac{J}{E_b} dV_{b2}} \;\square\cdots$$

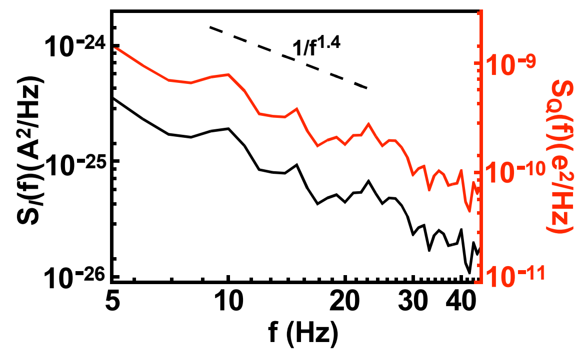
Here dV_{b1} and dV_{b2} come from the electrodes and the background.

Charge/Gate Noise-Induced Dephasing



$S_V(\omega) = 3\times 10^{-10}\ \mathrm{V}^2/\omega$

Based on data from H.W. Liu

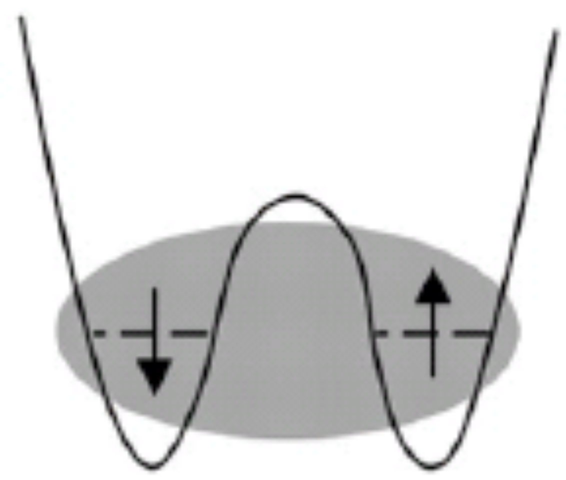


RTN noise: $$\frac{\rho_{12}(t)}{\rho_{12}(0)} = e^{-t/\tau}\left(\cos\,\eta t + \frac{1}{\eta\tau}\sin\,\eta t\right)$$

1/f noise: $$\begin{cases} \rho_{12}(t)/\rho_{12}(0) = e^{-\chi(t)} \\ \chi(t) = \dfrac{1}{2\hbar^2}\left(\dfrac{dJ}{dV}\right)^2 \displaystyle\int_{\omega_0}^{\infty} d\omega S_V(\omega)\left(\dfrac{\sin\,\omega t/2}{\omega/2}\right)^2 \end{cases}$$

D. Culcer, X. Hu, and S. Das Sarma, APL **95**, 073102 (2009).

How Are Two-Spin States in a Double Dot Affected by Electron-Phonon Interactions



$$|S\rangle = \frac{1}{\sqrt{2}}\left[\psi_L(1)\psi_R(2) + \psi_L(2)\psi_R(1)\right]$$

$$\times \frac{1}{\sqrt{2}}\left(|\uparrow\rangle|\downarrow\rangle - |\downarrow\rangle|\uparrow\rangle\right)$$

$$|T\rangle_0 = \frac{1}{\sqrt{2}}\left[\psi_L(1)\psi_R(2) - \psi_L(2)\psi_R(1)\right]$$

$$\times \frac{1}{\sqrt{2}}\left(|\uparrow\rangle|\downarrow\rangle + |\downarrow\rangle|\uparrow\rangle\right)$$

➢The two-electron singlet and triplet states have **different charge distributions**. The **phonons** will therefore couple to them differently.

Dephasing of Two-Spin States in the Presence of Phonon Relaxation

Take a simple model of generic exponential phonon relaxation (lattice anharmonicity, electron-phonon int., phonon leakage) with a single rate for all phonons. Then

$$\rho_{ST}(t)=\rho_{ST}(0)\,e^{-B_1^2(t)-B_2^2(t)}$$

where

$$B_1^2(t)=\frac{V}{2(2\pi)^3}\int d^3\vec{q}\,\frac{\left|g(\vec{q})\right|^2}{\omega_q^2\left(\omega_q^2+\gamma^2/4\right)^2}\coth\frac{\hbar\omega_q}{2k_BT}$$

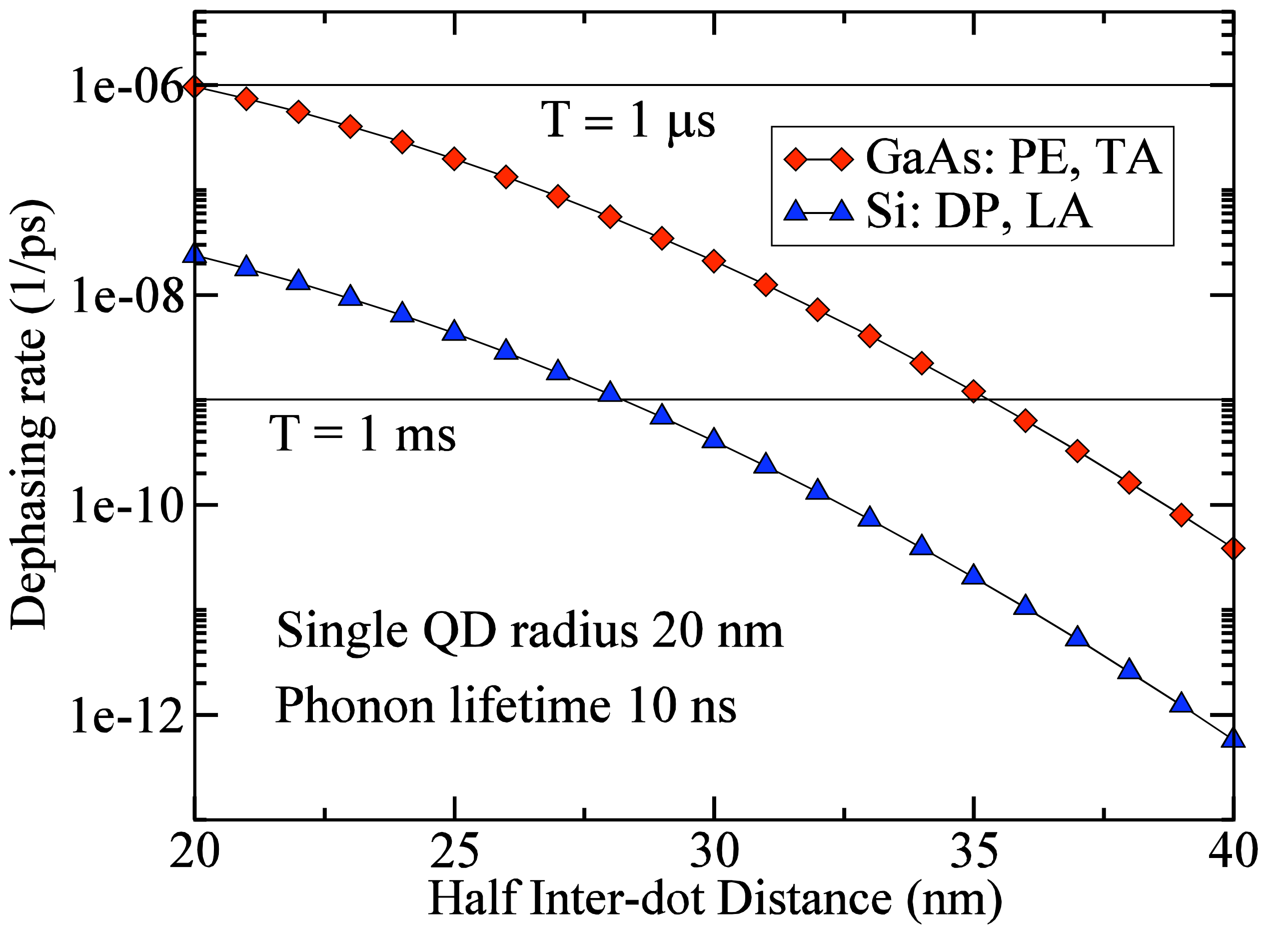
$$\times\left[\left(\omega_q^2-\gamma^2/4\right)\left(1-e^{-\gamma t/2}\cos(\omega_q t)\right)-\frac{\gamma\omega_q}{2}e^{-\gamma t/2}\sin(\omega_q t)\right]$$

$$B_2^2(t)=\frac{\gamma t}{2}\frac{V}{2(2\pi)^3}\int d^3\vec{q}\,\frac{\gamma\left|g(\vec{q})\right|^2}{\omega_q^2\left(\omega_q^2+\gamma^2/4\right)^2}\coth\frac{\hbar\omega_q}{2k_BT}\equiv\Gamma_{ST}t$$

$B_2^2(t)$ **is an exponential decay term that originates from phonon decay:**

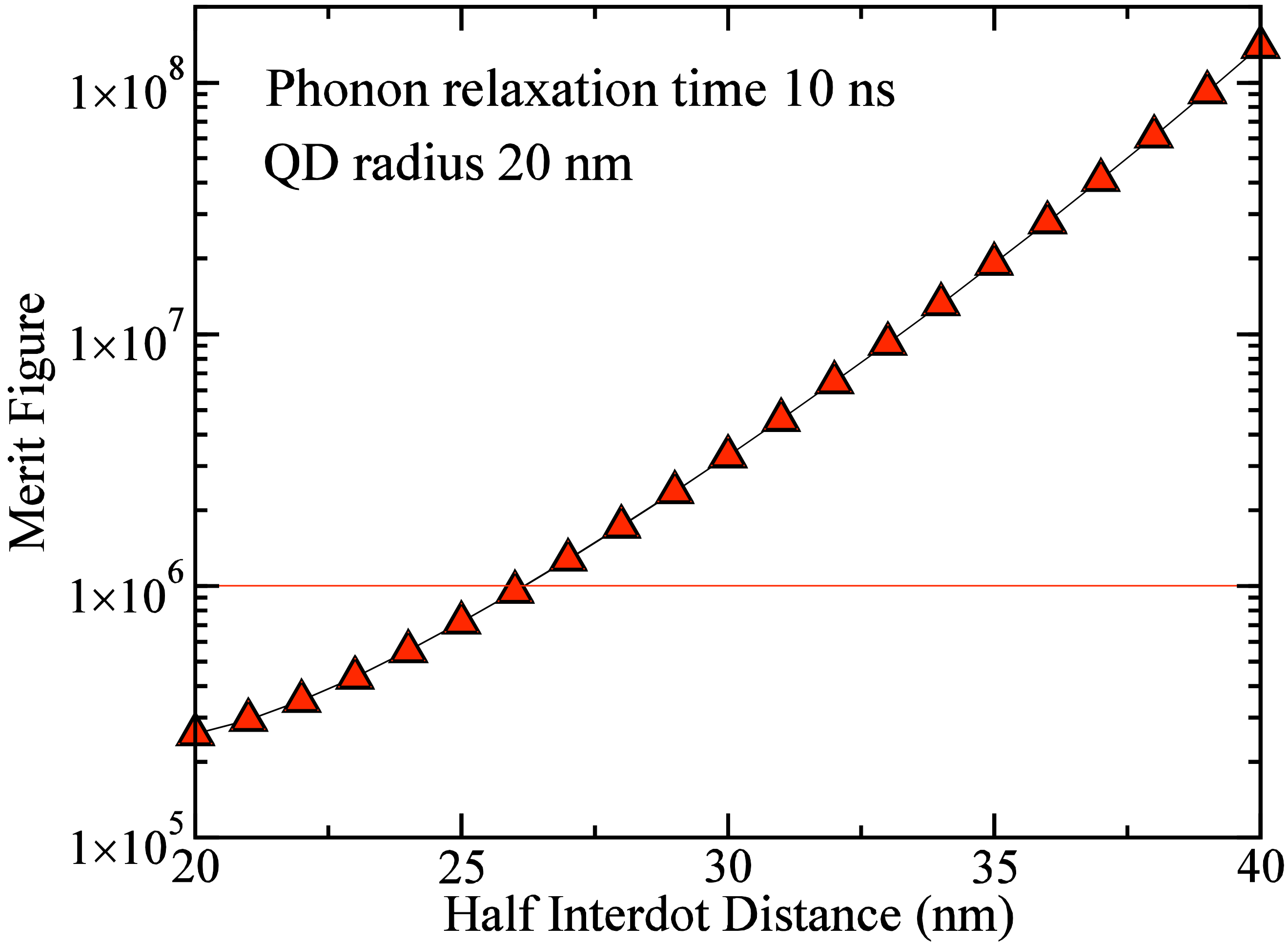
$$\rho_{ST}(t)=\rho_{ST}(0)\,e^{-\Gamma_{ST}t-B_1^2(t)}$$

Two-Spin Dephasing through Electron-Phonon Interaction



- Si about two orders of magnitude better than GaAs.

Two-Spin Dephasing: Merit Figure



For this calculation here we use GaAs parameters.

Additional Questions on the Phonons

- For **biased double dot**, charge distribution difference between singlet and triplet states would acquire an electrical dipole component---should increase phonon-induced dephasing.

- **Optical phonon** induced dephasing effect needs to be evaluated: optical phonons generally have much shorter lifetime (in the order of 10 ps).

- …

Summary

- Hyperfine interaction very weak in Si QDs. Spin coherence time should be very long;

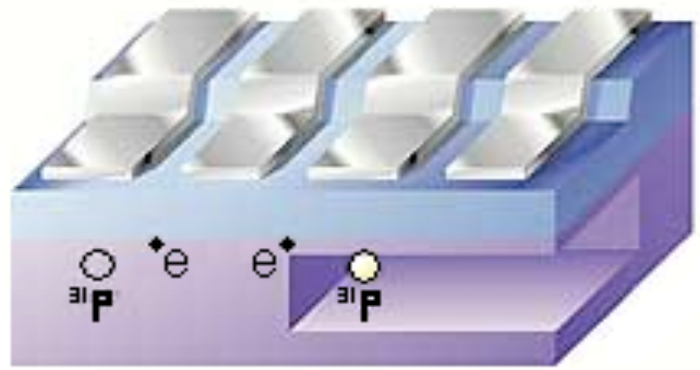
- When two spins are exchange coupled, effect of charge noise could be important;

- When two spins are exchange coupled, phonons can also cause decoherence, and phonon relaxation leads to exponential decay, though its magnitude is generally small;

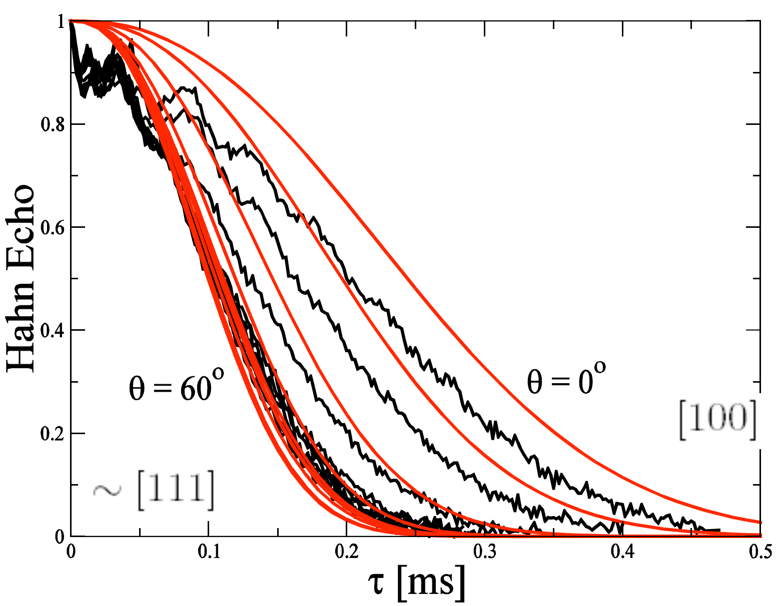
- …

Hyperfine Interaction in Si:P

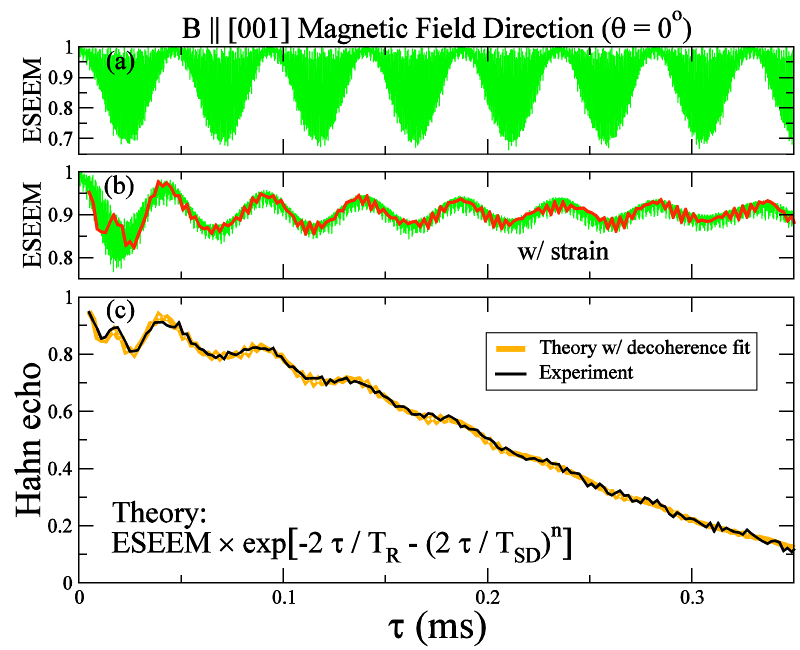
- Decoherence of donor electron spin in Si:P well understood;
- Spectral diffusion due to ^{29}Si nuclear spins in the environment dominates;
- Anisotropic hyperfine coupling causes ESEEM;
- Hyperfine coupling matrix well



Kane, Nature (98); Vrijen etal, PRA (00).

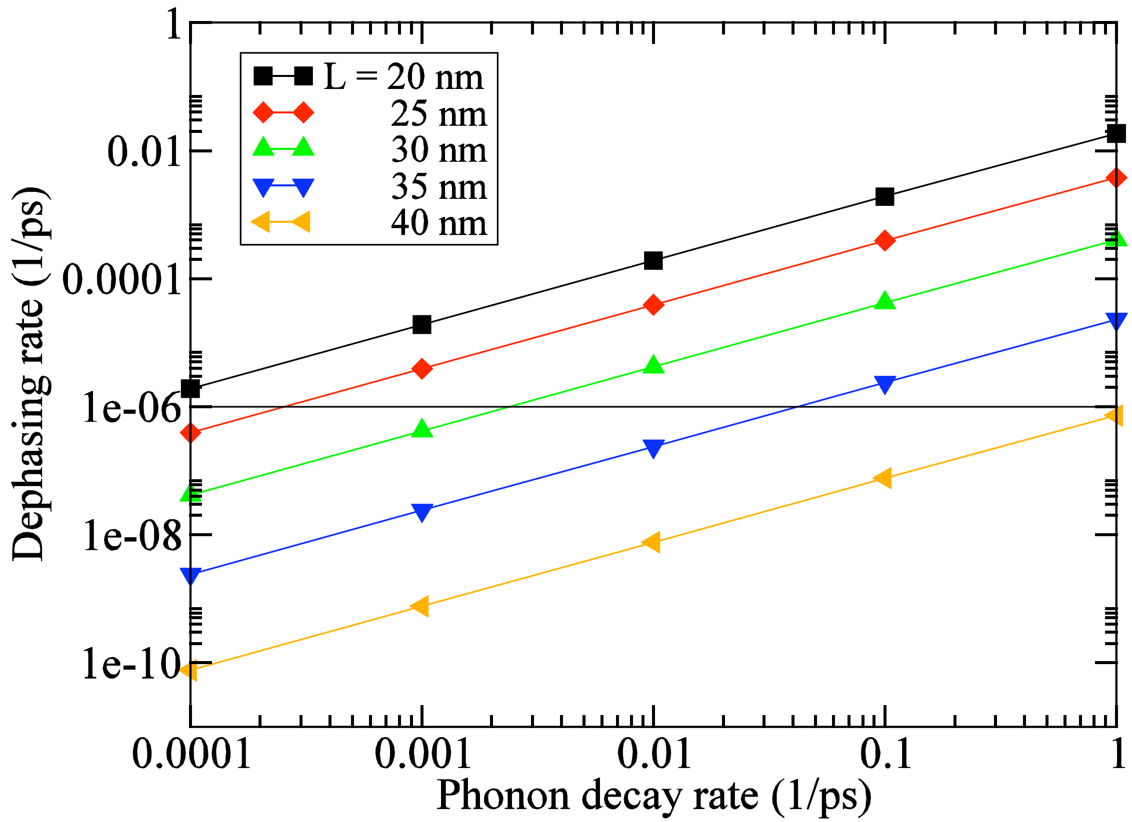


W. Witzel et al, PRB (06).



W. Witzel et al, PRB (07).

Two-Spin Dephasing by TA Phonons via Piezoelectric Interaction in GaAs



$$\Gamma_{ST} = \frac{\hbar^2}{2}\,\frac{V}{2(2\pi)^2\hbar^2}\int d^3\vec{q}\;\frac{\left|g(\vec{q})\right|^2}{(\omega_q-\omega)^2+(\gamma/2)^2}\coth\frac{\hbar\omega_q}{2k_BT}$$